An Index Analysis from Coupled Circuit and Device Simulation

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1 Introduction

Nowadays the semiconductor devices in an electrical circuit are modelled by equivalent circuits containing basic network elements described by algebraic and ordinary differential equations. But the correct adjustment of these circuits has become a very difficult task for the network design. In [1] a new model for electrical circuits containing semiconductor devices is proposed. There the differential algebraic equations (DAEs) for the basic circuit's elements are coupled to partial differential equations (PDEs), more specifically to one-dimensional Drift-Diffusion (DD) equations, modelling the semiconductor devices in it. Systems of this type are called Abstract Differential Algebraic Systems (ADAS). In [7] the tractability index [4] of this model is analysed and in [6] it is proved that the DAE obtained after discretization in space of the DD equations in it has the same index as the abstract system. In this work we study the index of an abstract system where higher dimensional PDEs describe the behavior of the semiconductor devices in the circuit. In the next section the model is briefly described. The section 3 is devoted to the study of the index of the system, as ADAS. Finally, in section 4 it is shown that the index of the DAE that is obtained after discretization in space of the PDEs is equal to the index of the abstract system. In what follows we consider electrical circuits with only one semiconductor device, the results can easily be generalized to circuits containing more semiconductor devices.

2 Abstract Differential Algebraic System for the simulation of electrical circuits

Suppose Ω is a bounded domain in $\mathbb{R}^d,\ d \in \{1,2,3\}$, $x \in \Omega$ represents the space variable and t is the time variable, $t \in [t_0,\, t_F]$. The system proposed in [7] for the simulation of electrical circuits containing semiconductor devices couples the Modified Nodal Analysis (MNA) equations for electrical circuits to the DD equations for semiconductor devices.

The MNA equations for an electrical circuit have the form

$$A_C \frac{\mathrm{d}\, q_C(A_C^T e, t)}{\mathrm{d}t} + A_R g(A_R^T e, t) + A_L j_L + A_V j_V + A_S j_S + A_I i_S = 0, \quad (1a)$$

$$\frac{\mathrm{d}\, \phi(j_L, t)}{\mathrm{d}t} - A_L^T e = 0, \quad (1b)$$

$$A_V^T e - v_S = 0, \quad (1c)$$

where A_C, A_R, A_L, A_V, A_S and A_I are the element related reduced incidence matrices, $v_S(t)$, $i_S(t)$, $q_C(u,t)$, $g(u,t)$ and $\phi(j,t)$ are given functions and the unknowns are the node potentials, excepting the mass node $e(t): \mathbb{R} \to \mathbb{R}^{n_N}$ and the currents through inductors, voltage sources and semiconductor devices $j_L(t): \mathbb{R} \to \mathbb{R}^{n_L}$, $j_V(t): \mathbb{R} \to \mathbb{R}^{n_V}$ and $j_S: \mathbb{R} \to \mathbb{R}^{n_S}$ respectively. The DD equations are given by the following set of PDEs for the electrostatic potential $\psi(x,t)$ and the electrons and holes densities, $n(x,t)$ and $p(x,t)$ respectively

$$\nabla \cdot (-\varepsilon \nabla \psi) - q(C - n + p) = 0, \quad (1d)$$

$$-\frac{\partial n}{\partial t} + \frac{1}{q}\mathrm{div} J_n - R = 0, \quad J_n - q\mu_n(U_T \nabla n - n \nabla \psi) = 0, \quad (1e)$$

$$\frac{\partial p}{\partial t} + \frac{1}{q}\mathrm{div} J_p + R = 0, \quad J_p + q\mu_p(U_T \nabla p + p \nabla \psi) = 0. \quad (1f)$$

We consider $R = R(n,p), \mu_n = \mu_n(x), \mu_p = \mu_p(x)$ and ε, q and U_T as constants. In (1d)-(1f), as suggested in [3], we replace the Poisson equation (1d) by the energy conservation equation

$$\nabla \cdot (J_n + J_p - \varepsilon \partial_t \nabla \psi) = 0, \quad (1g)$$

obtained after differentiation of (1d) with respect to time and elimination of $\frac{\partial n}{\partial t}$ and $\frac{\partial p}{\partial t}$ from the continuity equations (1e) and (1f).

We consider the boundary of the semiconductor device to be divided in two disjoint parts $\Gamma = \Gamma_O \cup \Gamma_A$. The first one are the metal semiconductor contacts (Ohmic contacts) where the external potentials are applied and the second one is an artificial boundary. The boundary conditions are

$$n = n_D(x), \; p = p_D(x), \; \psi = \psi_{bi}(x) + \psi_D(x, e) \quad \text{on } \Gamma_O \quad (1h)$$

$$\text{and } \frac{\partial \psi}{\partial \nu} = \frac{\partial n}{\partial \nu} = \frac{\partial p}{\partial \nu} = 0 \quad \text{on } \Gamma_A, \quad (1i)$$

where ψ_D denotes the externally applied bias, it depends on the node potentials of the circuit.

Suppose $\Gamma_O = \cup_{j=1}^{n_S+1} \Gamma_j$. The current flowing through the contact $\Gamma_i \subset \Gamma_O$ of the semiconductor is $j_i = \int_{\Gamma_i} J_{tot} \cdot \nu \mathrm{d}\sigma$ where $J_{tot} = J_n + J_p - \varepsilon \frac{\partial}{\partial t} \nabla \psi$. If $f(x) = (f_1(x) \; f_2(x) \; \ldots \; f_{n_S}(x))$ is such that

$$\Delta f_i = 0 \text{ in } \Omega, \quad f_i|_{\Gamma_j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{else} \end{cases}, \; j = 1, 2, \ldots, n_S + 1, \quad (\nabla f_i \cdot \nu)|_{\Gamma_A} = 0, \tag{1j}$$

the current through $\Gamma_i,\ i = 1, 2, \ldots, n_S$ can be calculated as [3]

$$j_i = \int_{\Gamma_i} J_{tot} \cdot \nu \,\mathrm{d}s = \int_{\Gamma} J_{tot} \cdot \nu f_i \,\mathrm{d}s = \int_{\Omega} J_{tot} \cdot \nabla f_i \mathrm{d}x$$
$$j_i = -\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega} \nabla\psi \cdot \nabla f_i \mathrm{d}x + \int_{\Omega} (J_n + J_p) \cdot \nabla f_i \mathrm{d}x.$$

The current at Γ_{n_S+1} is the negative sum of the currents through the other contacts[1]. Suppose the contact Γ_i of the semiconductor device is joined to the k_i-th node of the circuit for $i = 1, 2, \ldots, n_S + 1$. We set $\psi_D(x, e) = e_{k_i} - e_{k_{n_S+1}}\ \forall x \in \Gamma_i,\ i = 1, 2, \ldots, n_S$, and $\psi_D(x, e) = 0,\ \forall x \in \Gamma_{n_S+1}$. Then according to the definition of A_S in [7], $\psi_D(x, e) = f(x) \cdot A_S^T e$. Following the convention in [2] the vector j_S must be such that

$$j_{S_i} = -j_i = -\int_{\Omega} (J_n + J_p) \cdot \nabla f_i \mathrm{d}x + \frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega} \varepsilon \nabla\psi \cdot \nabla f_i \,\mathrm{d}x, \; i = 1, 2, \ldots, n_S$$
$$j_{S_i} = -\int_{\Omega} (J_n + J_p) \cdot \nabla f_i \mathrm{d}x - \frac{\mathrm{d}}{\mathrm{d}t} j^d_{S_i}, \quad j^d_{S_i} = -\int_{\Omega} \varepsilon \nabla\psi \cdot \nabla f_i \,\mathrm{d}x. \tag{1k}$$

Let the following assumptions on the circuit equations be satisfied in the forthcoming sections:

1. the input functions $v_S(t)$ and $i_S(t)$, associated to the independent voltage and current sources respectively, are continuous,
2. the functions $q_C(u, t)$, $\phi(j, t)$ and $g(u, t)$ are continuously differentiable and have positive definite partial Jacobians
$$C(u, t) = \frac{\partial q_C(u, t)}{\partial u}, \quad L(j, t) = \frac{\partial \phi(j, t)}{\partial j}, \quad G(u, t) = \frac{\partial g(u, t)}{\partial u},$$
3. the circuit contains neither loops of voltage sources only nor cut sets of current sources only. These two conditions hold if and only if the matrices A_V and $(A_C\ A_R\ A_L\ A_V\ A_S)^T$ have full column rank, respectively,
4. the function $R(n, p)$ is continuously differentiable,
5. the functions $\mu_n(x)$ and $\mu_p(x)$ are bounded.

3 Tractability index of the Abstract Differential Algebraic System

If $u = \big(e,\, j_L,\, j_V,\, j_S,\, j^d_S,\, \psi(\cdot, t),\, n(\cdot, t),\, p(\cdot, t)\big)$ the above described model, after homogenization of the electrostatic potential and the densities of electrons

[1] The sum of the currents at the contacts of the semiconductor is zero, $\sum_{i=1}^{n_S+1} j_i = \sum_{i=1}^{n_S+1} \int_{\Gamma_i} J_{tot} \cdot \nu \mathrm{d}s = \int_{\Gamma} J_{tot} \cdot \nu \mathrm{d}s = \int_{\Omega} \nabla \cdot J_{tot} \mathrm{d}x = 0$.

and holes [2], can be written as $\mathcal{A}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}(u,t)+\mathcal{B}(u,t)=0$ with

$$\mathcal{A}=\begin{pmatrix} A_C & 0&0&0&0&0 \\ 0 & I&0&0&0&0 \\ 0&0&0&0&0&0 \\ 0&0&0&0&0&0 \\ 0&0&I&0&0&0 \\ 0&0&0&I&0&0 \\ 0&0&0&0&I&0 \\ 0&0&0&0&0&I \end{pmatrix}, \mathcal{B}(u,t)=\begin{pmatrix} A_R g(A_R^T e,t)+A_L j_L+A_V j_V+A_S j_S+A_I i_s(t) \\ -A_L^T e \\ A_V^T e - v_S(t) \\ j_S^d+\varepsilon\begin{pmatrix} \int_\Omega \nabla\left(\psi+f\cdot A_S^T e\right)\cdot\nabla f_1 \mathrm{d}x \\ \vdots \\ \int_\Omega \nabla\left(\psi+f\cdot A_S^T e\right)\cdot\nabla f_{n_S} \mathrm{d}x \end{pmatrix} \\ j_S+\begin{pmatrix} \int_\Omega (J_n+J_p)\cdot\nabla f_1 \mathrm{d}x \\ \vdots \\ \int_\Omega (J_n+J_p)\cdot\nabla f_{n_S} \mathrm{d}x \end{pmatrix} \\ \nabla\cdot(J_n+J_p) \\ \frac{1}{q}\nabla\cdot J_n - R \\ \frac{1}{q}\nabla\cdot J_p + R \end{pmatrix} \quad (2a)$$

and

$$\mathcal{D}(u,t)=\left(A_C^+ A_C q_C(A_C^T e,t),\ \phi(j_L,t),\ j_S^d,\ \nabla\cdot(-\varepsilon\nabla\psi),\ -n,\ p\right)^T. \quad (2b)$$

In (2) $J_n=q\mu_n\left(U_T\nabla(n+g_2)-(n+g_2)\nabla\left(\psi+f\cdot A_S^T e+g_1\right)\right)$, J_p has a similar structure and A_C^+ is the Moore-Penrose pseudo-inverse of A_C. $\mathcal{A},\mathcal{D}$ and $\mathcal{B}$ are operators acting on Hilbert spaces $\mathcal{A}:\mathcal{Z}\to\mathcal{Y}$, $\mathcal{D}:\mathcal{X}\to\mathcal{Z}$ and $\mathcal{B}:\mathcal{X}\to\mathcal{Y}$ with

$$\begin{aligned} \mathcal{X}&=\mathbb{R}^{n_N}\times\mathbb{R}^{n_L}\times\mathbb{R}^{n_V}\times\mathbb{R}^{n_S}\times\mathbb{R}^{n_S}\times V\times L^2(\Omega)\times L^2(\Omega), \\ \mathcal{Y}&=\mathbb{R}^{n_N}\times\mathbb{R}^{n_L}\times\mathbb{R}^{n_V}\times\mathbb{R}^{n_S}\times\mathbb{R}^{n_S}\times L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega), \\ \mathcal{Z}&=\mathbb{R}^{n_C}\times\mathbb{R}^{n_L}\times\mathbb{R}^{n_S}\times L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega), \end{aligned}$$

where $V=\left\{v\in H^2(\Omega)\,|\,v|_{\Gamma_O}=0, (\nabla v\cdot\nu)|_{\Gamma_A}=0\right\}$. Note that the definition domain $\mathcal{D}_\mathcal{B}$ of $\mathcal{B}(u,t)$,

$$\mathcal{D}_\mathcal{B}=\mathbb{R}^{n_N}\times\mathbb{R}^{n_L}\times\mathbb{R}^{n_V}\times\mathbb{R}^{n_S}\times\mathbb{R}^{n_S}\times V\times V\times V,$$

is dense in $\mathcal{X}$. The Fréchet derivative of $\mathcal{D}(u,t)$ is

$$\mathcal{D}_0(u,t)=\begin{pmatrix} A_C^+ A_C C(A_C^T e,t)A_C^T & 0 & 0\,0\,0 & 0 & 0 & 0 \\ 0 & L(j_L,t) & 0\,0\,0 & 0 & 0 & 0 \\ 0 & 0 & 0\,0\,I & 0 & 0 & 0 \\ 0 & 0 & 0\,0\,0 & -\varepsilon\Delta & 0 & 0 \\ 0 & 0 & 0\,0\,0 & 0 & -I & 0 \\ 0 & 0 & 0\,0\,0 & 0 & 0 & I \end{pmatrix}$$

and because the equation $-\varepsilon\Delta u=f$, completed with homogeneous Dirichlet and Neumann conditions, has a unique solution for all $f\in L^2(\Omega)$,

$$\begin{aligned} \operatorname{im}\mathcal{D}_0(u,t)&=\operatorname{im}A_C^T\times\mathbb{R}^{n_L}\times\mathbb{R}^{n_S}\times L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega), \\ \ker\mathcal{D}_0(u,t)&=\left\{w\in\mathcal{X}\mid w_e\in\ker A_C^T, w_L=0, w_S^d=0, w_\psi=0, w_n=0, w_p=0\right\}. \end{aligned}$$

[2] $\psi=\psi-f(x)\cdot A_S^T e-g_1(x)$ where $g_1(x)$ is such that $(\nabla g_1\cdot\nu)|_{\Gamma_A}=0$, $g_1|_{\Gamma_O}=\psi_{bi}(x)$, $n=n-g_2$ where g_2 is such that $(\nabla g_2\cdot\nu)|_{\Gamma_A}=0$, $g_2|_{\Gamma_O}=n_D$ and $p=p-g_3$ where g_3 is such that $(\nabla g_3\cdot\nu)|_{\Gamma_A}=0$, $g_3|_{\Gamma_O}=p_D$.

On the other hand, the operator $\mathcal{A}$ satisfies

$$\ker \mathcal{A} = \ker A_C \times \{0\} \times \{0\} \times \{0\} \times \{0\} \times \{0\},$$
$$\operatorname{im} \mathcal{A} = \operatorname{im} A_C \times \mathbb{R}^{n_L} \times \{0\} \times \{0\} \times \mathbb{R}^{n_S} \times L^2(\Omega) \times L^2(\Omega) \times L^2(\Omega).$$

The coupled system has a properly stated leading term because

$$\ker \mathcal{A} \oplus \operatorname{im} \mathcal{D}_0(u,t) = \mathcal{Z}, \quad \forall u \in \mathcal{X},\ \forall t \in [t_0, t_F]$$

and there is a projector $\mathcal{R} \in \mathcal{L}(\mathcal{Z})$[3] such that $\operatorname{im} \mathcal{R} = \operatorname{im} \mathcal{D}_0(u,t)$, $\ker \mathcal{R} = \ker \mathcal{A}$[4].

Remark *The functions $f_1, f_2, \dots f_{n_S}$ defined above are a basis of the linear space*

$$\mathcal{F} = \left\{ v \in H^2(\Omega) \mid \Delta v = 0 \text{ in } \Omega,\ (\nabla v \cdot \nu)|_{\Gamma_A} = 0,\ v|_{\Gamma_j} = a_j,\ v|_{\Gamma_{n_S+1}} = 0 \right\},$$

where $j = 1, 2, \dots, n_S$ and $a_j \in \mathbb{R}\ \forall j$. Because $(u,v)_{\mathcal{F}} = \int_\Omega \nabla u \cdot \nabla v\, dx$ is a scalar product in $\mathcal{F}$, the matrix

$$J = \begin{pmatrix} \int_\Omega \nabla f_1 \cdot \nabla f_1\, dx & \dots & \int_\Omega \nabla f_1 \cdot \nabla f_{n_S}\, dx \\ \vdots & \vdots & \vdots \\ \int_\Omega \nabla f_{n_S} \cdot \nabla f_1\, dx & \dots & \int_\Omega \nabla f_{n_S} \cdot \nabla f_{n_S}\, dx \end{pmatrix}, \tag{3}$$

is positive definite.

Theorem 1. *If the conditions on the circuit mentioned in section 2 are satisfied and the circuit contains neither cut sets of inductors and current sources (LI-cut sets) nor loops of capacitors, voltage sources and semiconductor devices with at least one voltage source or one semiconductor device (CVS-loops), the abstract system has tractability index one.*

Proof: Let $\mathcal{G}_0(u,t) = \mathcal{A}\mathcal{D}_0(u,t)$ and $\mathcal{B}_0(u,t)$ denote the Fréchet-derivative of $\mathcal{B}$. Under the conditions in section 2 $\mathcal{B}_0(u,t)$ exists. The system has tractability index one if there is a projection operator $\mathcal{Q}_0 \in \mathcal{L}(\mathcal{X})$ onto $\ker \mathcal{G}_0(u,t)$ such that $\mathcal{G}_1(u,t) = \mathcal{G}_0(u,t) + \mathcal{B}_0(u,t)\mathcal{Q}_0$ is injective and $\operatorname{im} \mathcal{G}_1(u,t) = \mathcal{Y}$ for all $u \in \mathcal{X}$ and $t \in [t_0, t_F]$.

Because the system has a properly stated leading term, $\ker \mathcal{G}_0(u,t) = \ker \mathcal{D}_0(u,t)$ and $\mathcal{Q}_0 = \begin{pmatrix} Q_C & 0&0&0&0&0&0&0 \\ 0 & 0&0&0&0&0&0&0 \\ 0 & 0&I&0&0&0&0&0 \\ 0 & 0&0&I&0&0&0&0 \\ 0 & 0&0&0&0&0&0&0 \\ 0 & 0&0&0&0&0&0&0 \\ 0 & 0&0&0&0&0&0&0 \\ 0 & 0&0&0&0&0&0&0 \end{pmatrix}$ is a projection operator onto

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[3] $\mathcal{L}(\mathcal{Y})$ denotes the space of linear operators $A : \mathcal{Y} \to \mathcal{Y}$.

[4] $\mathcal{R} = \begin{pmatrix} A_C^+ A_C & 0&0&0&0&0 \\ 0 & I&0&0&0&0 \\ 0 & 0&I&0&0&0 \\ 0 & 0&0&I&0&0 \\ 0 & 0&0&0&I&0 \\ 0 & 0&0&0&0&I \end{pmatrix}$.

$\ker \mathcal{G}_0(u,t)$ if Q_C is a projector onto $\ker A_C^T$. The operator $\mathcal{G}_1$ can easily be calculated. Let $w = \left(w_e, w_L, w_V, w_S, w_S^d, w_\psi, w_n, w_p\right) \in \ker \mathcal{G}_1(u,t)$. The fourth equation of $\mathcal{G}_1(u,t)w = 0$ is $\varepsilon J A_S^T Q_C w_e = 0$ where J is the matrix in (3), then $\varepsilon J A_S^T Q_C w_e = 0$ iff $A_S^T Q_C w_e = 0$. The sixth equation of $\mathcal{G}_1(u,t)w = 0$ is $-\varepsilon \Delta w_\psi = 0$, it implies that $w_\psi = 0$. The rest of the proof is very similar to the ones in [7] or in [6]. We arrive to

$$\begin{aligned}\ker \mathcal{G}_1(u,t) = \Big\{ w \mid w_\psi = 0, w_n = 0, w_p = 0, Q_C w_e \in \ker \left(A_C\ A_R\ A_V\ A_S\right)^T, \\ P_C w_e = -H_C(\cdot)^{-1} \left(A_V \quad A_S\right) \left(\begin{smallmatrix} w_V \\ w_S \end{smallmatrix}\right), w_L = L(\cdot)^{-1} A_L^T Q_C w_e, \\ \left(\begin{smallmatrix} w_V \\ w_S \end{smallmatrix}\right) \in \ker \left(Q_C^T A_V\ Q_C^T A_S\right), w_S^d = -\left(0 \quad I\right) \left(\begin{smallmatrix} w_V \\ w_S \end{smallmatrix}\right) \Big\},\end{aligned}$$

where $H_C(A_C^T e, t) = A_C C(A_C^T e, t) A_C^T + Q_C^T Q_C$ is positive definite. If the circuit contains neither LI-cut sets ($(A_C\ A_R\ A_V\ A_S)^T$ has full column rank) nor CVS-loops with at least one voltage source or one semiconductor device ($\left(Q_C^T A_V\ Q_C^T A_S\right)$ has full column rank), then $\ker \mathcal{G}_1(u,t) = \{0\}$, i.e. $\mathcal{G}_1(u,t)$ is injective. The dense solvability of $\mathcal{G}_1(u,t)$ ($\overline{\operatorname{im} \mathcal{G}_1(u,t)} = \mathcal{Y}$) can be shown using similar arguments as those in [7] and taking into account that J is nonsingular $\square$.

Suppose the circuit contains LI-cut sets or CVS-loops with at least one voltage source or one semiconductor device. Let Q_{CRVS} be a projector onto $\ker \left(A_C\ A_R\ A_V\ A_S\right)^T$ and Q_{C-VS}, a projector onto $\ker \left(Q_C^T A_V\ Q_C^T A_S\right)$. Because $\operatorname{im} Q_{CRVS} \subset \operatorname{im} Q_C$, Q_{CRVS} can be constructed so that $\ker Q_C \subset \ker Q_{CRVS}$. A projector $\mathcal{Q}_1(u,t)$ onto $\ker \mathcal{G}_1(u,t)$ is then

$$\mathcal{Q}_1(u,t) = \begin{pmatrix} Q_{CRVS} & 0 & -H_C(\cdot)^{-1}(A_V\ A_S) Q_{C-VS} & 0 & 0 & 0 & 0 \\ L(\cdot)^{-1} A_L^T Q_{CRVS} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & Q_{C-VS} & 0 & 0 & 0 & 0 \\ 0 & 0 & -(0\ I) Q_{C-VS} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Theorem 2. *Under the conditions mentioned in section 2 and if the circuit contains LI-cut sets or CVS-loops, the coupled system has tractability index two.*

Proof: The ADAS has index two if the operator $\mathcal{G}_2(u,t) = \mathcal{G}_1(u,t) + \mathcal{B}_0(u,t)(I - \mathcal{Q}_0)\mathcal{Q}_1(u,t)$ is injective and densely solvable for all $u \in \mathcal{X}$ and $t \in [t_0, t_F]$.

The operator $\mathcal{G}_2(u,t)$ can easily be calculated. Let w be an element in $\ker \mathcal{G}_2(u,t)$. The third and fourth equations of $\mathcal{G}_2(u,t)w = 0$, pre-multiplied by Q_{C-VS}^T, can be written as

$$-Q_{C-VS}^T \left\{ \begin{pmatrix} A_V^T \\ A_S^T \end{pmatrix} H_C(\cdot)^{-1} \left(A_V\ A_S\right) + \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{\varepsilon} J^{-1} \end{pmatrix} \right\} Q_{C-VS} \left(\begin{smallmatrix} w_V \\ w_S \end{smallmatrix}\right) = 0. \quad (4)$$

Because $\begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{\varepsilon} J^{-1} \end{pmatrix}$ is positive semidefinite and $H_C^{-1}(\cdot)$ is positive definite, equation (4) is satisfied iff $Q_{C-VS} \left(\begin{smallmatrix} w_V \\ w_S \end{smallmatrix}\right) = 0$. The rest of the proof is very similar to the ones in [7] or in [6]. We arrive to $\ker \mathcal{G}_2(u,t) = \{0\}$. The dense solvability of $\mathcal{G}_2(u,t)$ can be proved following the lines in [7] $\square$.

4 Index of the Discrete System

Suppose that the coupled system, after discretization in space of the Drift-Diffusion equations has the following form

$$A_C \frac{\mathrm{d}\, q_C(A_C^T e, t)}{\mathrm{d}t} + A_R g(A_R^T e, t) + A_L j_L + A_V j_V + A_S j_S + A_I i_S = 0, \quad (5a)$$

$$\frac{\mathrm{d}\, \phi(j_L, t)}{\mathrm{d}t} - A_L^T e = 0, \quad (5b)$$

$$A_V^T e - v_S = 0, \quad (5c)$$

$$j_S^d + J_h A_S^T e + g(y) = 0, \quad (5d)$$

$$j_S + j_S^c(A_S^T e, y, t) + \frac{\mathrm{d}\, j_S^d}{\mathrm{d}t} = 0, \quad (5e)$$

$$A \frac{\mathrm{d}\, y}{\mathrm{d}t} + b(A_S^T e, y, t) = 0, \quad (5f)$$

where A is a nonsingular matrix and J_h is positive definite. The vector y is $y = (\Psi,\, N,\, P)^T$ and Ψ, N and P define the approximations to $\psi(x,t)$, $n(x,t)$ and $p(x,t)$ by the discretization method. Then, in a similar way as in the previous section it can be shown that its index is always less or equal to two and it is two only if the circuit contains LI-cut sets or CVS-loops.

4.1 The Scharfetter-Gummel discretization of the Drift-Diffusion equations

If the so-called Scharfetter-Gummel Discretization is applied to the DD equations in (2) the resulting DAE has the same structure as (5). The Scharfetter-Gummel scheme can be described as a Finite Element Method for the discretization of the Drift-Diffusion equations that is based on the assumption that the current densities J_n and J_p are constant on each element (triangles, tetrahedrons, etc) of the spatial mesh. For a detailed description of this method we refer to [5].

Suppose $\mathcal{T} = \{T_1,\, T_2,\, \ldots,\, T_K\}$ is a conforming triangulation of Ω and $\mathcal{P} = \{P_1,\, P_2,\, \ldots,\, P_M,\, \ldots,\, P_N\}$ denotes the set of vertices of elements in $\mathcal{T}$, where $P_i \in \Omega \cup \Gamma_A$ for $i = 1, 2, \ldots, M$. Let $\{\varphi_1,\, \varphi_2,\, \ldots,\, \varphi_N\}$ be continuous functions that are linear on each $T_i \in \mathcal{T}$ and satisfy $\varphi_i(P_j) = \begin{cases} 1, \text{ if } i = j \\ 0, \text{ else} \end{cases}$.
The coefficients that define the approximation $\psi_h(x,t) = \sum_{j=1}^N \Psi_j(t)\varphi_j(x)$ are given by

$$\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} \sum_{T \ni P_i} \sum_{j=1}^{N} \Psi_j \int_T \nabla\varphi_j \cdot \nabla\varphi_i \,\mathrm{d}x - \int_\Omega (J_n + J_p) \cdot \nabla\varphi_i \,\mathrm{d}x = 0, \qquad (6)$$

where $i = 1, 2, \ldots, M$. The last $N - M$ values of Ψ_j are $\Psi_j = \psi_{bi}(P_j) + f_h(P_j) \cdot A_S^T e$ where $f_h = (f_{1,h},\, f_{2,h},\, \ldots,\, f_{n_S,h})$ are approximations to the functions f_i defined in (1j). Suppose the functions $f_{i,h}$ are calculated as $\sum_{j=1}^{N} f_{i,h}(P_j)\varphi_j(x)$. If we substitute $\Psi_j,\ j = M+1,\ M+2,\ \ldots,\ N$ in (6) by their values and introduce the change of variables $\tilde{\Psi}_j = \Psi_j - f_h(P_j) \cdot A_S^T e,\ j = 1, 2, \ldots, M$[5] the following equations are obtained

$$\sum_{T \ni P_i} \sum_{j=1}^{M} \tilde{\Psi}_j \int_T \nabla\varphi_j \cdot \nabla\varphi_i \,\mathrm{d}x - \int_\Omega (J_n + J_p) \cdot \nabla\varphi_i \,\mathrm{d}x = 0. \tag{7a}$$

The discretized continuity equations are

$$-\frac{\mathrm{d}}{\mathrm{d}t} \sum_{T \ni P_i} \int_T n\varphi_i \,\mathrm{d}x - \frac{1}{q} \int_\Omega J_n \cdot \nabla\varphi_i \,\mathrm{d}x - \int_\Omega R\varphi_i \,\mathrm{d}x = 0, \tag{7b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{T \ni P_i} \int_T p\varphi_i \,\mathrm{d}x - \frac{1}{q} \int_\Omega J_p \cdot \nabla\varphi_i \,\mathrm{d}x + \int_\Omega R\varphi_i \,\mathrm{d}x = 0, \tag{7c}$$

where $i = 1, 2, \ldots, M$. If the integrals involving derivatives with respect to the time of n and p are approximated by a quadrature formula the system (7) has the form $A\frac{\mathrm{d}y}{\mathrm{d}t} + b(A_S^T e, y, t) = 0$ where A is a nonsingular matrix and $y = \left(\tilde{\Psi}, N, P\right)^T$. The equations for j_S^d can be written as $j_{S_i}^d + \varepsilon J_h A_S^T e + g(\tilde{\Psi}) = 0$ with a positive definite matrix J_h that has the same form as (3) but with the functions $f_{i,h}(x)$ instead of $f_i(x)$.

References

1. G. Ali, Bartel A., Günther M., Tischendorf C.: Elliptic Partial Differential Algebraic Multiphysics Models in Electrical Network Design, Math. Models Meth. Appl. Sci., **13(9)**, pp. 1261–1278, (2003).
2. Chua L. O., Desoer C. A., Kuh E. S.: Linear and Nonlinear Circuits. McGraw-Hill Book Company, (1987).
3. Gajewski H.: Analysis und Numerik von Ladungstransport in Halbleitern, Technical Report, Weierstrass Institut für Andgewandte Analysis und Stochastik, **6**, (1993).
4. Lamour R., März R., Tischendorf C.: PDAEs and Further Mixed Systems as Abstract Differential Algebraic Systems, Technical Report, Institute of Mathematics, Humboldt University of Berlin, **11**, (2001).
5. Markowich, P.: The stationary Semiconductor Device Equations, Springer Verlag, (1986).
6. Selva Soto, M., Tischendorf C.: Numerical analysis of DAEs from coupled circuit and semiconductor simulation, APPNUM, to appear.
7. Tischendorf C.: Coupled Systems of Differential Algebraic and Partial Differential Equations in Circuit and Device Simulation, Habilitation Thesis, Humboldt University of Berlin, Berlin (2003).

[5] The (tractability) index of a DAE is invariant under regular variable transformations.